Bayesian Analysis of Nuclear Energy-Density Functional from Densities

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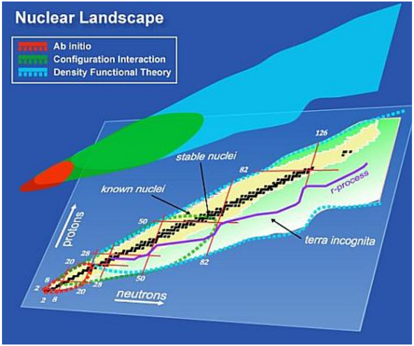
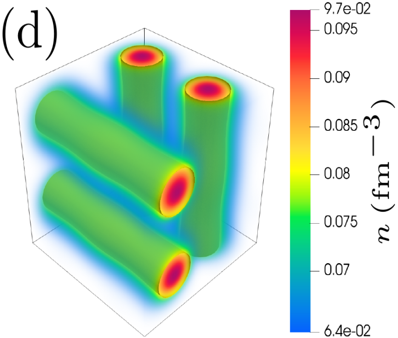
2026.7.15

Symposium on Nuclear Structure, Reaction, and Astrophysics (NuSRAP2026)

Background I

Energy-Density Functional (EDF): unified description of finite nuclei and bulk nuclear matter.





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Background II

Parameters of EDF, e.g.,

$$e[\rho] = \sum_t \Big[(C^{\rho}_{t0} + C^{\rho}_{tD}\rho^{\gamma})\rho_t^2 + C_t^{\Delta\rho}\rho_t \Delta\rho_t + C_t^{\tau}\rho_t\tau_t + C_t^{\nabla J}\rho_t \nabla\cdot \boldsymbol{J}_t + \dots \Big], \tag{1}$$

$t = 0, 1$: isoscalar/isovector.

- Fixed by experimental observables using point-like optimization (χ^2 test) e.g.,
  - masses and radii of doubly magic nuclei, fission barriers
  - equation of state for neutron matter
  - ...
- A few Bayesian studies in recent years*

* E.g., 10.1103/PhysRevC.111.014311

Background III

Rapid development of ab initio calculations.

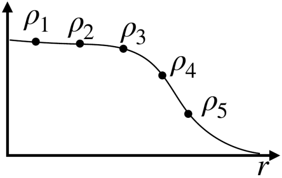
- Project **Quantum Matter Science in the Universe Opened Up by Precise Numerical Calculations**
  - Accurate ab-initio calculation of beyond-10-body quantum many-body systems based on nuclear forces.
- Compare to experiments. . .
  - Access data difficult to access in experiments (e.g., $\rho_n(r)$);
  - Small error bars.

Very interesting to determine EDF parameters from ab initio results. . .

Purpose

Establish the following framework

1. **Input**:
   - $(r_i,\ \rho_{ni},\ \rho_{pi})$ of light nuclei
   - Ground state energies E_{tot}.



2. **Method**: Bayesian analysis
3. **Output**: Skyrme parameters
4. **Prediction**
   - Nuclear matter properties.
   - Density profile of heavy nuclei.

Method I

Bayesian analysis:

$$P(\theta, \sigma_\rho, \sigma_E | X, Y) \propto P(X, Y | \theta, \sigma_\rho, \sigma_E) P(\theta, \sigma_\rho, \sigma_E). \tag{2}$$

posterior $\propto$ likelihood $\times$ prior

- $\theta =$ (Skyrme parameters), dim$\theta = 10$,
- σ_ρ, σ_E: noise parameters, explained later
- Input data $X = \{(r_i, \rho_{ni}, \rho_{pi}) | i = 0, 1, 2, \cdots\}$ for different nuclei,
- Input data $Y = E_{tot}$ for different nuclei.

So far, no ab initio X...for the nuclei we want to use...
Use $(r_i.\rho_{ni}, \rho_{pi})$ generated by EDF instead.

Method II

Likelihood: density

$$P(X|\theta,\sigma_\rho) = \prod_{(N,Z)} \frac{1}{2\pi\sigma_\rho^2} e^{-\frac{\|X - X_\theta\|^2}{2\sigma_\rho^2}}. \tag{3}$$

X_θ: $\rho_{n\theta}(r)$, $\rho_{p\theta}(r)$ predicted by the Skyrme EDF with parameter set θ, calculated using the HFBRAD code* (modified)

The distance between X and X_θ:

$$\|X - X_\theta\|^2 = \sum_{t=n,p} \left(\frac{\sum_i |\rho_{ti} - \rho_{t\theta}(r_i)| \rho_{ti} r_i^2}{\sum_i \rho_{ti} r_i^2} \right)^2. \tag{4}$$

* See arxiv nucl nucl-th/0501002

Method III

Likelihood: energy

$$P(Y|\theta,\sigma_E) = \prod_{(N,Z)} \frac{1}{\sqrt{2\pi\sigma_E^2}} e^{-\frac{|Y-Y_\theta|^2}{2\sigma_E^2}}. \tag{5}$$

Method IV

Prior

Uniform prior of $\theta = (C^{\rho}_{t0}, C^{\rho}_{tD}, C^{\Delta\rho}_{t}, C^{\tau}_{t}, C^{\nabla J}_{t}, \gamma)^T$ does not work!

- Strongly correlated, bad numerical performance.
- No direct physical interpretation.

Method V

Strategy: choose θ indirectly from nuclear matter parameters.
Phenomenological model of nuclear matter

$$E = E_0 + \frac{1}{2} K_0 \left(\frac{\rho - \rho_0}{3\rho_0} \right)^2 + \left[J + L \left(\frac{\rho - \rho_0}{3\rho_0} \right) + \frac{1}{2} K_{\mathrm{sym}} \left(\frac{\rho - \rho_0}{3\rho_0} \right)^2 \right] \left(\frac{\rho_n - \rho_p}{\rho_0} \right)^2 . \tag{6}$$

Parameters: ρ_0, E_0, K_0, J, L.

Method VI

Additional parameters:

- **Effective masses** m_s^*, m_v^*.
- **Spin-orbit parameter** W_0.

One-to-one mapping*:

C_{t0}^{ρ}, C_{tD}^{ρ}, $C_t^{\Delta\rho}$, C_t^{τ}, $C_t^{\nabla J}$, γ $\longleftrightarrow$ ρ_0, E_0, K_0, J, L, $C_t^{\Delta\rho}$, m_s^*, m_v^*, W_0

* See 10.1103/PhysRevC.80.014322, 10.1103/PhysRevC.82.024321, 10.1103/PhysRevC.111.014311.

Method VII

Uniform prior for the nuclear matter parameters*:

- $\rho_0 = 0.150\text{–}0.175\,\mathrm{fm}^{-3}$,
- $E_0 = -16.50\text{–}-15.50\,\mathrm{MeV}$,
- $K_0 = 180\text{–}260\,\mathrm{MeV}$,
- $J = 25.00\text{–}37.00\,\mathrm{MeV}$,
- $L = 10\text{–}120\,\mathrm{MeV}$,
- $C_0^{\Delta\rho} = -120\text{–}-20\,\mathrm{MeV}\cdot\mathrm{fm}^5$,
- $C_1^{\Delta\rho} = -50\text{–}50\,\mathrm{MeV}\cdot\mathrm{fm}^5$,
- $W_0 = 80.00\text{–}170.00\,\mathrm{MeV}\cdot\mathrm{fm}^5$,
- $m_0 = (0.70\text{–}1.10)m$, $m = 938.92\,\mathrm{MeV}$,
- $m_1 = (0.60\text{–}0.90)m$.

$*$ Follow the suggestion of (10.1103/PhysRevC.111.014311).

Method VIII

Additional constrain: dimensional analysis of χEFT*,

$$\bar{C} = s f_\pi^{2(l-1)} \Lambda^{n+l-2} \hbar^m C, \tag{7}$$

$$C = C_{t0}^{\rho},\ C_{tD}^{\rho},\ C_t^{\Delta\rho}, C_t^{\tau}, C_t^{\nabla J}. \tag{8}$$

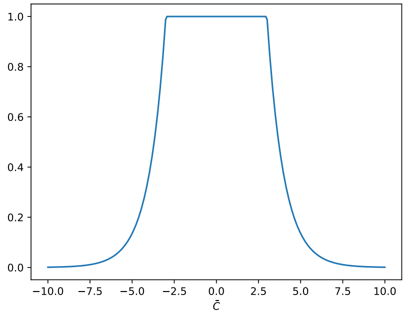
$$f_\pi = 93\,\mathrm{MeV}, \Lambda = 687\,\mathrm{MeV}. \tag{9}$$

- s=1 if isoscalar else 4
- l=2+γ if C_{tD}^{ρ} else 2
- n=0 if C_{t0}^{ρ} or C_{tD}^{ρ} else 2
- m=3 if C_{t0}^{ρ}, $3 + 3\gamma$ if C_{tD}^{ρ} else 5

$*$ M. Kortelainen, 2010 10.1103/PhysRevC.82.011304

Method IX

	Couplings in natural units				
	SIII	HFB16	Average	Min.	Max.
C_{00}^{ρ}	-0.4767	-0.7759	-0.7977	-1.2380	-0.4465
C_{10}^{ρ}	1.2076	1.9295	1.7656	-0.9795	4.5761
$C_{0\mathrm{D}}^{\rho}$	0.7623	0.7509	0.7824	0.2723	1.2616
$C_{1\mathrm{D}}^{\rho}$	-3.0493	-2.3825	-2.2010	-6.0116	1.9790
C_{0}^{τ}	0.6059	0.4464	0.5606	-0.0856	2.9421
C_{1}^{τ}	-1.6726	-0.2048	-0.3626	-2.9469	3.5160
$C_{0}^{\Delta\rho}$	-0.8597	-0.8702	-0.8765	-1.7491	-0.4636
$C_{1}^{\Delta\rho}$	0.9301	-0.8998	-0.5531	-15.5202	2.5762
$C_{0}^{\nabla J}$	-1.2288	-1.4449	-1.2385	-1.6384	-0.8957
$C_{1}^{\nabla J}$	-1.6384	-1.9265	-1.0875	-2.1846	5.4272
C_{0}^{J}	0	1.1300	0.5159	-0.6021	1.4212
C_{1}^{J}	0	1.3208	1.6502	-5.0026	3.6049



$C_{00}^{\rho} < 0$, $C_{0D}^{\rho} > 0$, $C_{0}^{\Delta\rho} < 0$, $C_{t}^{\nabla J} < 0$

(final prior) $=$ (nuclear matter part) $\times$ (χEDF part)

Method X

Final unknown parameter: σ_ρ, σ_E.
Empirical prior of σ:

$$\sigma_\rho \sim \frac{2}{\sqrt{2\pi\sigma_\rho'^2}} e^{-\frac{\sigma_\rho^2}{2\sigma_\rho'^2}}, \qquad \sigma_\rho > 0 \tag{10}$$

$$\sigma_E \sim \frac{2}{\sqrt{2\pi\sigma_E'^2}} e^{-\frac{\sigma_E^2}{2\sigma_E'^2}}, \qquad \sigma_E > 0 \tag{11}$$

$$\sigma_\rho' = 0.1 \times (0.16\,\mathrm{fm}^{-3}),\ \sigma_E' = 1.00\,\mathrm{MeV} \tag{12}$$

Method XI

10D-θ space, no naive computation of $P(\theta, \sigma_\rho, \sigma_E | X, Y)$...

Algorithm: Metropolis-Hastings sampling

1. Define an empty sample set $S = \{\}$.
2. Choose initial $\theta^{(0)}$, $\sigma_{\rho,E}^{(0)}$.
3. Choose $\theta^{(1)} = \theta^{(0)} + \delta\theta$, $\delta\theta \sim \mathcal{N}(0, s^2)$, $\sigma^{(1)} = \sigma_{\rho,E}^{(0)} + \delta\sigma_{\rho,E}$, $\delta\sigma_{\rho,E} \sim \mathcal{N}(0, s'^2)$.
4. Compute acceptance rate

$$\alpha = \frac{P(\theta^{(1)}, \sigma_\rho^{(1)}, \sigma_E^{(1)} | X, Y)}{P(\theta^{(0)}, \sigma_\rho^{(0)}, \sigma_E^{(0)} | \rho, E)} \tag{13}$$

Method XII

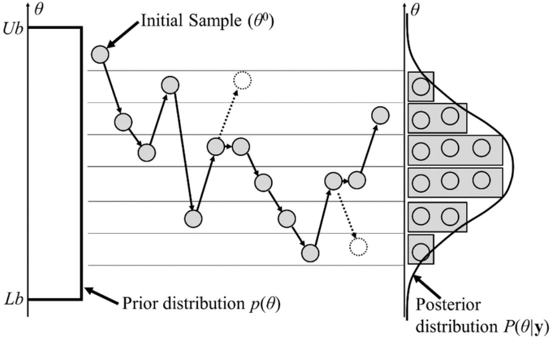
5. Define $\alpha' \sim \text{uniform}(0,1)$. If $\alpha' < \alpha$,
   - add $\left(\theta^{(1)}, \sigma_{\rho,E}^{(1)}, P(\theta^{(1)}, \sigma_{\rho}^{(1)}, \sigma_{E}^{(1)}|\rho, E)\right)$ to S;
   - $\theta^{(0)} \leftarrow \theta^{(1)}$, $\sigma_{\rho,E}^{(0)} \leftarrow \sigma_{\rho,E}^{(1)}$.
6. Go to step 3.

Method XIII

Output: Sample set

$$\left\{ \left(\theta^{(k)}, \sigma_{\rho,E}^{(k)}, P(\theta^{(k)}, \sigma_{\rho}^{(k)}, \sigma_{E}^{(k)} | X, Y) \right) | k = 0, 1, 2, \cdots \right\} \tag{14}$$

$$P(\theta, \sigma_{\rho}, \sigma_{E} | X, Y) \propto (\text{density of samples}). \tag{15}$$



Method XIV

Representative parameters

- Maximum A Posteriori (MAP)

$$k_{\mathrm{MAP}} = \mathrm{argmax}_k P(\theta^{(k)}, \sigma_\rho^{(k)}, \sigma_E^{(k)} | X, Y), \tag{16}$$

$$\theta_{\mathrm{MAP}} = \theta^{(k_{\mathrm{MAP}})} \tag{17}$$

- Gaussian Model: fit the samples with

$$P(\theta) = \frac{1}{\sqrt{(2\pi)^N \det \Sigma}} e^{-\frac{1}{2}(\theta-\mu)^T \Sigma^{-1}(\theta-\mu)}, \tag{18}$$

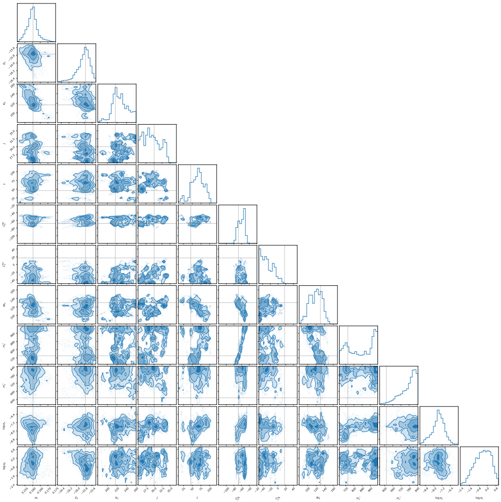
$$\theta_{\mathrm{G}} = \mu \pm (\mathrm{diag}\,\Sigma)^{1/2}. \tag{19}$$

Results I

Setup

- Input nuclei: ^{16}O, ^{40}Ca, ^{48}Ca
- $(r_i, \rho_{ni}, \rho_{pi})$ number: 3×100
  Randomly distributed on $0 < r < 10\,\mathrm{fm}$
- Add noise to the input data: no
- EDF used to produce input: SkM*
- Final sample size: $\sim 10^4$
- Prediction target: ^{208}Pb

Results II



Grey line: accurate results.

Results III

Fitting quality

$\|\rho_n - \rho_{n,\theta}\|$ (fm^{-3})

(N,Z)	Gaussian	MAP
(8,8)	0.000142	0.000017
(20,20)	0.000219	0.000090
(28,20)	0.000519	0.000159

$\|\rho_p - \rho_{p,\theta}\|$ (fm^{-3})

(N,Z)	Gaussian	MAP
(8,8)	0.000141	0.000033
(20,20)	0.000223	0.000067
(28,20)	0.000406	0.000307

$|E_{tot} - E_{tot,\theta}|$ (MeV)

(N,Z)	Gaussian	MAP
(8,8)	1.587	0.068
(20,20)	2.228	0.012
(28,20)	1.854	0.043

$$\|\rho - \rho_\theta\| = \frac{\sum_i |\rho_{ti} - t(r_i)|\rho_{ti} r_i^2}{\sum_i \rho_{ti} r_i^2}. \tag{20}$$

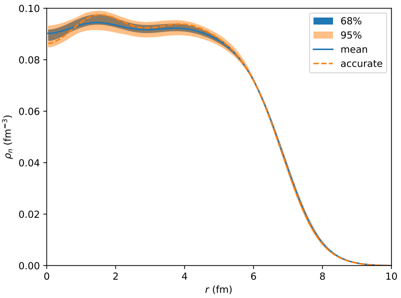
Results IV

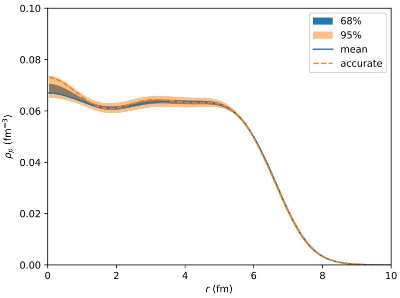
Prediction: nuclear matter

Name	accurate	Gaussain	MAP
ρ_0	0.160	0.160$\pm$0.004	0.161
E_0	-15.770	-15.821$\pm$0.167	-15.771
K_0	216.596	226.648$\pm$15.722	216.287
J	30.033	29.262$\pm$2.564	25.571
L	45.778	65.306$\pm$18.603	47.186

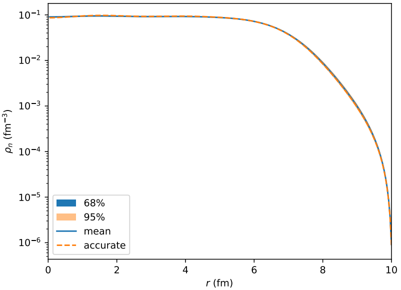
Results V

Prediction: ^{208}Pb

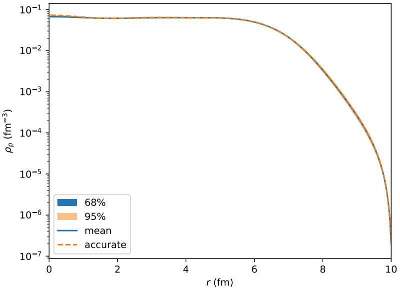




Results VI



10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
ρ_n (fm^{-3})
0
2
4
6
8
10
r (fm)
68%
95%
mean
accurate



10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
10^{-7}
ρ_p (fm^{-3})
0
2
4
6
8
10
r (fm)
68%
95%
mean
accurate

Results VII

$E_{tot}(\text{accurate}) = -1626.550\,\mathrm{MeV}$
$E_{tot}(\text{mean}) = -1633.098\,\mathrm{MeV}$
$E_{tot}(68\%) = -1653.691$ – $-1628.636\,\mathrm{MeV}$
$E_{tot}(95\%) = -1668.992$ – $-1612.193\,\mathrm{MeV}$

Summary

Topic: fixing Skyrme parameters from densities.

Method: Bayesian analysis

Current status: The model

- finds parameters fitting nicely with input;
- predicts nuclear matter and ^{208}Pb properties.

Next step: improve the sampling speed.